

Freshman Research Initiative Virtual Drug Screening (VDS) Syllabus Spring 2015

Course Uniques:

BIO	102C	CONFERENCE COURSE-FRI	47820
BIO	206L	LAB EXP BIO: STRC/FUNC ORG-FRI	48030
CH	204	INTRO TO CHEMICAL PRACT-FRI	50285 – Primary for Canvas
CH	108	CONFERENCE COURSE-FRI	50630

Stream Principal Investigator (PI):

Dr. Jon Robertus
WEL 5.266

Research Educator (RE):

Dr. Josh Beckham - 'Dr. B'
PAI 3.04H
Office Hours: **anytime**

471-5022 (office)

Teaching Assistant(s):

Oscar
Melissa

Mentors & Researchers:

Maria (**Charina**)
Andrea (**Andee**)
Cidia
Nicole (**Nikki**)
Xenia (**Brianna**)
Avery
Alberto
John

Research Guru: **Luis**

Meeting Times & Class Locations:

Class:

BUR 216, Tues, 3:30 - 4:30pm

Lab:

PAI 2.14, Times are variable

Computer Labs:

WEL 2.144 (East One) WEL 2.128 (North One)

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Course Overview

This course includes both wet labs and computational/computer-based labs to teach you the skills necessary to find novel drugs against various diseases, pathogens and toxins. The wet lab portion of the course will take place in PAI 2.14. You will be learning basic wet lab techniques that are important in a research environment as well as specific techniques for our research. By the end of the semester you will be competent in preparing solutions, spectrophotometry, and protein expression, purification and characterization of purity and yield. On the virtual side, you will be able to analyze 3 dimensional structures of macromolecules, interface remotely with a High Performance cluster computer to carry out computational screening, and assess small molecule binding to a target based upon the output of a molecular docking program.

Computer labs will initially be spent learning how to visualize and analyze protein structures and protein-ligand interactions through the program PyMol (<http://www.pymol.org/>). PyMol is available on the computers in the Welch Hall Computer Lab (WEL 2.144). You are encouraged to install the free academic version available on the Schrödinger website on your own computer and become familiar with the use of the program. Instructions on the use of PyMol form the basis of the first three computer labs while molecular docking programs will be used in the later labs to carry out virtual screening. Lab time will be scheduled in WEL 2.144 and/or WEL 2.128, but some of the work can be performed independently.

Spring 2015 Experiment Schedule:

Wk	Start Date (Mon)	Experiment	Assignment
1	1/19 - Mon	Introduction, Lab tours and lab safety walk throughs, Lab: Precision & Accuracy	Online Lab Safety Lab Pre-Q's (due each week)
2	1/26	Lab: Buffers & Solutions (No lab report – only notebook) -- Start your Mini Research write up	Lab Notebook Lab Safety Videos
3	2/2	Lab: Pymol lab 1 -- Continue Mini Research write up,	Mini Res Write up Lit Assign, Bibliography (EndNote) Assign TA meetings
4	2/9	Lab: Beer's Law	Lab Notebook Beer's Law Lab report TA meetings
5	2/16	Lab: Pymol lab 2 & Transformation starts	Peer review for Beer's Law Report Wiki Posting of Mini Res Write Up
6	2/23	Lab: Bacterial protein expression	Lab Notebook
7	3/2	Lab: Pymol lab 3 & Purification starts	TA meetings Final Version of Beer's Law Report
8	3/9	Lab: Protein purification	Lab Notebook
9	3/16	No lab (spring break)	
10	3/23	Lab: Virtual Screening 1	Lab report
11	3/30	Lab: Protein characterization	TA meetings Lab Notebook
12	4/6	Lab: Virtual Screening Phosphatase (YopH & FtHap)	Combined Lab Report of 3 protein labs
13	4/13	Lab: Target Discovery Exercise (Buffer Titration Demos)	Lab Notebook
14	4/20	Lab: Enzyme Assay	TA meetings
15	4/27	Lab:	
16	5/4	Class and Lab Cleanup	Final Lab report Lab Notebook

Quantitative Reasoning Flag:

This course carries the Quantitative Reasoning flag. Quantitative Reasoning courses are designed to equip you with skills that are necessary for understanding the types of quantitative arguments you will regularly encounter in your adult and professional life. You should therefore expect a substantial portion of your grade to come from your use of quantitative skills to analyze real-world problems.

<http://www.utexas.edu/ugs/flags/students/about/quantitative-reasoning>

Meeting Times:

The weekly class meetings are mandatory. The lecture portion will provide the theoretical background for the lab and helpful hints and details on how to perform the experiments, proper use of equipment, and data interpretation. You are expected to take notes during the class since most of the material is not contained in a textbook or the handouts.

The times in lab are also mandatory but the time will vary based upon the given experiment. If you cannot make a class meeting or the lab, then you need to contact the RE in advance.

You are required to **sign in** when you come to lab so that we have a record of your work (in binder near door). You are also required to have a mentor, TA, or RE check you out each time you leave the lab. This is to verify that you have left your lab space clean, which counts towards your Lab Conduct grade.

Team Meeting Times:

Each student will be a part of a Team of 3-5 other students along with a Mentor that will lead the group. Your team will meet weekly or every other week for about 30 min to 1 hour to discuss the labs and make sure you are confident in your understanding of the material and what you are doing in lab. The mentors will help you to understand how the lab fits in the overall research and what to expect in the weeks ahead.

Office Hours:

You can always make appointments with the RE for help and discussion outside of the allotted lab times. The mentors and the TA may be contacted via e-mail with quick questions outside of lab but they are not obligated to spend extensive time in this manner. Consequently, you may be referred to the RE.

Course Communication:

- Announcements, course handouts and protocols will be available via handouts, email or posted on Canvas and/or on [Google Docs](#). You are expected to check your email and Canvas on a regular (daily basis) for any pertinent course communication. Class slides will be posted to online a few days after each class.
- Face to face, email, text and phone are all acceptable methods of contacting the RE.
- A wiki/blog page will be used as part of the Mini Research Assignment to share information amongst the class about the various targets. (Wikispaces)
 - NOTE: When you create an account for Wikispaces, use your first name and last initial for the login. e.g. joshb. If you have the same first name and last initial as someone else - then the next letter in your last name e.g. joshbe

Scheduling:

We will keep track of scheduling in the labs by using Google calendar. For the Painter lab, we will use the calendar to show when mentors, the TA or the RE will be present. We may also use it to reserve certain pieces of equipment (e.g. PCR machines, spectrophotometers) if it gets too crowded.

Google Calendar for the VDS class

Login:

The Painter lab should be open from 9 AM to 9 PM every weekday. There will also be some hours on Saturday and/or Sunday which are yet to be determined.

You can only work in the lab if a **mentor** or **TA** or **RE** is present! This is for safety reasons.

Course Assessment

Since this course is not a typical Lab course, the course will also be evaluated on a different basis. You will learn that in research, experiments don't always work. Sometimes you might follow the protocol but still not get expected results. Science is a process of trial and error, as long as you learn from your failure it is a success. You are expected to understand the theoretical background of the techniques you are using and to keep a good record

of what was done in the Lab. This will be recorded in your Lab notebook and summarized in a weekly Lab report for evaluation.

Course Weighting:

Lab notebook	30%
Lit. Search Assign. + Bibliography	2%
Mini Research Write up + Wiki Page	8%
Lab reports	30%
Quizzes, TA Meetings, In class and misc. assignments	14%
Final Lab report	10%
Lab Conduct/effort + Lab Safety	6%
Total	100%

NOTE: Late assignments will lose **5%** of their total value per day

Plus/minus Grading:

The Virtual Drug Screening stream will take advantage of the plus/minus grading system for your final grade in the class, wherein:

A = 4.0, A- = 3.67, B+ = 3.33, B = 3.0, B- = 2.67, C+ = 2.33
C = 2.0, C- = 1.67, D+ = 1.33, D = 1.0, D- = 0.67, F = 0.0

However, assignments during the course will be graded on a 10 point system, which will then be weighted by assignment and converted to the 4 point system at the end of the semester to calculate your final grade:

(10, 9.75, 9.5, 9.25, 9.0, 8.75, 8.5, 8.25, 8.0, 7.75, etc..).

Grades may be curved at the end of the semester. You will be assessed on your abilities and effort amongst your classmates and upon your progress through the semester. An 'A' represents exemplary work beyond merely what has been assigned, an 'A-' represents completing everything that is asked in the class and understanding of the material, a 'B+' is for those that have missing or late assignments or are deficient in their understanding. 'B' is for those that have missing or late assignment and are deficient in understanding. Lower grades represent further degrees of the above.

Pre-Lab Questions/Quizzes:

Before each lab, a series of questions will need to be answered (either on paper or through Canvas). These will serve the purpose of getting you ready for the week ahead by having read through the lab protocol. You will be assessed on your effort. While having correct answers is best, we know that you won't always be able to have the correct solution since you haven't done the lab yet. During labs, you will be so busy with the procedures that we want you to be able to think about the concepts before you carry them out.

Lab Reports:

Reports are to be handed in or electronically submitted before our weekly class meetings unless otherwise notified. In addition, a **Final Lab report** that incorporates the last 2 labs will be due at the end of the semester. These reports will help you develop technical writing skills. Comments will be given and you will be graded on how your writing improves over the semester. Some reports will be combined and will count for their summed value of points.

Any work that is to be submitted electronically (via email or upload to Canvas or GoogleDocs) should have a descriptive filename so that it can be sorted easily. For example, name your file with

UTEID_Name_Date_AssignmentName.pdf

e.g. REF289_RosalindFranklin_Jan232015_Assignment1BuffersLab.pdf

NOTE: your **name, document title** and **page numbers** must be in the 'header' or 'footer' for all work submitted electronically. This is necessary so that when I print them out to write comments – I will know which pages belong to you! See the bottom of this page for an example.

e.g. “Rosalind Franklin Buffers & Solutions Lab

p. 3”

Lab Notebooks:

The detail and clarity of your notebook will be very important in conveying your understanding and effort.

A lab notebook grading rubric will be provided which will allow you to see exactly what needs to be included.

The notebook needs to be updated continuously as you perform experiments.

- You are required to write EVERYTHING pertaining to experiments in the lab notebook
- Graphs, spreadsheet data and images should be pasted into the lab notebook when appropriate
- Sketches and diagrams are encouraged!

Try to keep a sequential flow to the notebook, but when this is not possible then it is necessary to place page numbers so that you can refer to where an experiment picks up again. The RE will schedule lab notebook checks and randomly examine the individual notebooks through the semester as there is seldom a time to collectively evaluate them together.

- Lab notebooks must stay in the lab. You will not be allowed to take them home with you. So, plan to arrive early to start filling out your notebook before lab and then, if necessary, you can come in after your lab on another day to finish it up.
- Since the notebooks are property of the lab, they will be left with the stream at the end of the semester. It is your responsibility to make duplicates of protocols and data you wish to keep. Also, when you are writing your lab reports – you may want access to some of the information in your notebook. The best way to do this is to take pictures of your lab notebook pages beforehand.
- The wet lab entries must be handwritten, but computer labs (PyMol and Virtual Screening) can be pasted in from a WORD document that you will have created while in the computer lab (your work and modifications to protocol should be type in green/blue font). **Diagrams** and **sketches** are encouraged in your labnotebook – ‘a picture is worth a thousand words’

We require buying a lab notebook that is sturdy, can be written on both sides, large enough to paste graphs and figures into, and small enough to store easily in a drawer and not take up too much bench space when you are working in the lab

- Blueline notebooks (A9Q or A9, with or without grids, 192 pages costs \$5.95) from the COOP

The large carbon copy notebooks for some of the other chemistry course are NOT allowed – due to their size. Also, the ‘composition’ notebooks common for humanities classes are not permitted – they are too flimsy.

TA Meetings:

Approximately every other week, there will be individual meetings with each student and the TA and/or Dr. B. When someone is performing graduate work, they often have Committee Meetings that includes the professors that are on their Ph.D. committee. These meetings serve as progress check points to see if the candidate understands what they are doing and is still on track with their research. These are question and answer sessions but they are also times when the committee members can provide expert support to the students to help them along towards success. For VDS, these meetings will be a combination of the two. You will be asked questions by the TAs and Dr. B to assess your effort towards understanding of the concepts and materials in the work. You can also take the opportunity to ask questions back to the staff to clarify points of confusion or extend your knowledge about the science. Your grade for these will be based upon your accuracy but also your level of participation and effort.

Class Participation with TopHat®:

Participation in class discussion and responding to in-class questions will be a part of the overall grade. We will be using TopHat as a classroom response system in the VDS lecture time. Similar, to clickers - but better since you can use your own phone or device to respond. This will allow us to have a more effective in-class time for discussion and feedback. Note that there is a fee to the student of \$20 for a semester subscription to TopHat.

Lab Conduct/Effort:

You will be evaluated on a few basic principals of lab conduct that all good researchers (and workers in general) should possess:

1. **Enthusiasm:** How much desire the student has to learn the topics and apply them.
2. **Initiative:** How often a student proceeds independently on an experiment.
3. **Follow-through:** How well the student can complete an experiment correctly in a timely manner, once asked to.
4. **Absorptiveness:** How well the student understands the methods and can interpret data.
5. **Synthesis:** How well the student can develop new ideas and implement methods to new problems, design relevant experiments, and test those ideas.
6. **Writing/Organizational Ability:** How well the student can keep notebooks, explain or present ideas, describe the data and its meanings (reports), manage time, and express themselves.
7. **Cleanliness:** How well the student prevents contamination and cleans up after themselves. This will be evident in the experimental results and bench area. Be a good lab citizen.
8. **Collaboration:** How well the student collaborates with peers and communicates ideas effectively. This includes accurate descriptions of figures and the procedures they have done.

Please respect the equipment and keep it in good working order. You are expected to keep the area clean where you have carried out your experiments since this space is shared with three other VDS streams. Your lab grade will be partially dependent upon how well you cleanup after working in the lab and keeping the VDS supplies and reagents organized. A good habit to get in, is to try and clean at least one thing that is not yours before leaving the lab. This may simply be throwing away a loose tube on the floor or washing a piece of glassware. As you begin to work in smaller labs, your responsibility will increase and your cooperation will be appreciated even more by other lab members.

Organization**Materials:**

Tubes, plates, boxes, vials, bottles, and etc. must always be labeled appropriately or it will be discarded. In most cases you will use a short piece of colored tape to make a label. A complete label has the following information: VDS, Your Name (or initials), Date, Contents, Concentration, Experiment or sample number. All items should be labeled in 2 places: on the top and side. This is for redundancy for when one of the labels falls off or the ink is removed by a solvent.

Ice (not for human consumption) and autoclaves can be found in PAI 1.03. You are allowed to get ice on your own but autoclaving will be done by the mentors, TA or RE. Do not wear gloves in the hallway or outside the building.

Computers:

This course requires the use of computers for data collection, data analysis, and for communication purposes. We expect you to use your own data backup methods (UT Webspace: <http://webspace.utexas.edu/>, Gdrive, DropBox, or a thumb drive) to store all computer files generated. Some of the lab computers are re-imaged and are not a reliable place to store your files. It is your responsibility to have a back up of your data. PAI 2.14 has wireless access. Computer labs are available nearby in WEL 2.144 and ACA 1.126

Lab Safety Training

The following courses are required to be completed by the students enrolled in the Virtual Drug Screening stream. There is usually a short quiz that you must complete after each course. A copy of your training record must be printed out and submitted to the Research Educator (Dr. Beckham). The training record can be seen in TxClass by clicking on the 'Training History' link. This must be done before the first wet lab (Beer's Law) in PAI 2.14 (Painter Hall) is started.

DUE DATE: Prior to your Buffers & Solutions wet lab – bring printout to lab

General Info: Environmental Health and Safety Site for general information:

<http://www.utexas.edu/safety/ehs>

This course should have been completed by you in the fall Research Methods class— if not, do now:

OH 101 General Hazard Communication - online

<http://www.utexas.edu/safety/ehs/train/courses.html#oh101/>

These are the ones to be taken for Spring:

OH 102 Site Specific Hazard Communication - in person

To be completed in first week with Research Educator in the Painter 2.14 Lab.

This course may not show up in your Personal Training History for a week or so

OH 201 Laboratory Safety – online

<http://www.utexas.edu/safety/ehs/train/courses.html#oh201>

OH 202 Hazardous Waste Management – online

<http://www.utexas.edu/safety/ehs/train/courses.html#oh202>

OH207 biological safety training

<http://www.utexas.edu/safety/ehs/train/courses.html#oh207>

We will also need recombinant DNA training (**CW512**) through the IBC

https://utdirect.utexas.edu/cts/class.WBX?s_course_comp=0&s_course_prefix=CW&s_course_number=0512

FF205 Fire Extinguisher Training is not necessary for spring, but if you plan to stay for summer of fall, try to take the training this semester because it is only offered a few times.

<http://www.utexas.edu/safety/fire/extinguishers/training.html>

Verify your completion through Personal Training History:

<https://utdirect.utexas.edu/txclass/> (go to ‘Training History’)

There will also be several online videos and a Canvas quiz over safety which will need to be completed.

Safety & Waste Disposal

We may handle organic solvents (some may be highly corrosive to human skin and tissues) and other potentially dangerous chemicals and items. Safe lab practices and waste disposal procedures are mandatory and will be taught to you. Unsafe, imprudent and careless activities will result in you being removed from the lab. Continued noncompliance will result in a reduced lab grade and/or course failure. Please report anything you see that is unsafe (confidentially) to the TA or mentors.

1. Know the nearest location and proper use of the fire extinguisher (by both doors), first-aid kit and chemical spill-kit (both under the nanopure), eye-wash (middle sink).
2. Students must be supervised at all times while working in the laboratory.
3. Immediately report any accidents or mishaps to the mentors, TA, or RE.
4. You are required to wear latex or nitrile gloves when performing experiments. Know when to use latex vs nitrile. Also, know the location of safety glasses (cabinet) and lab coats (hanging on closet door next to entrance). Wear these safety items at all times especially when working with hazardous chemicals.
5. Always wear closed toed shoes and pants (NO SANDALS or SHORTS). Otherwise, you will have to wear booties and a lab coat or go home to change. You are welcome to keep a pair of clothes in a cubby to change into.
6. No food or beverages are allowed in the laboratory. PERIOD.
7. DO NOT store book bags on lab benches. They may go in the cabinets under the desks.
8. For your own safety and that of others, discard all waste appropriately:
 - a. Razor blades, needles, and other sharp METAL items should be placed in the Red plastic SHARPS containers
 - b. Glass must be placed in white cardboard boxes labeled “For Glass Disposal”.
 - c. Certain chemicals (PAGE and Phenol/Chloroform) must be placed in labeled waste containers in the chemicals hood.
 - d. Biologicals (bacteria) like LB agar plates must be placed in orange Biohazard waste containers for autoclaving. Liquid cultures must be killed with 10% bleach for 20 minutes and disposed down the center sink drain.

9. Glassware is to be washed promptly after use.
 - a. Remove ink or tape labels with ethanol
 - b. Scrub items with sponge or bottle brush and warm soapy water (Alconox – powder)
 - c. Triple rinse with tap water until soap is gone.
 - d. Inspect for cleanliness. If not clean, wash again.
 - e. Double rinse with distilled tap water.
 - f. Drain excess water in sink.
 - g. Invert all items to dry on peg boards or other designated locations for next class. Note, drying racks are provided for items that are easily tipped over. Once dry, replace to glassware cabinet.
10. The lab room should be as clean (or cleaner) when you leave, as it was when you arrived.
11. Report any problems or mishaps to your RE.

During certain laboratory exercises, you may be given special instructions regarding disposal of hazardous materials, chemical solutions such as organic solvent wastes, or biological material such as antibiotic-resistant bacteria. For your own safety and that of others, please follow these special directions carefully

ALWAYS ASK QUESTIONS BEFORE YOU DO SOMETHING IF YOU ARE UNSURE!

Accommodations

Please notify your instructors at the beginning of the semester of any modification/adaptation you may require to accommodate a disability-related-need. You will be requested to provide documentation to the Dean of Students' Office, in order that the most appropriate accommodations can be determined. Specialized services are available on campus through Services for Students with Disabilities (471-6259).

Appeals

The Research Educator, TA and Mentors will make decisions concerning grades, attendance and other policy matters. Should you disagree with a TA or Mentor, you are welcome to take the matter to the RE.

Academic Integrity

Policies for academic dishonesty are designed to help you and to be fair to the other individuals in the class. Scholastic dishonesty will not be tolerated. Being honest about your academic work is the foundation of your education. For this reason, cases of academic dishonesty will be regarded with the utmost seriousness whether this means copying someone else's Lab report or making up lab results. If quoting or paraphrasing from another source, please ask instructors, TA or mentors on the correct way to cite a reference. For a complete definition of unacceptable behavior, such as plagiarism, and the UT policy regarding such activities, see the Student Judicial Services website: http://deanofstudents.utexas.edu/sjs/acint_student.php.